



Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28014**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (neutral XH) 3.97
logP (X -) 1.86
RMSD 0.921

18B-28014 Points 2 to 29

M08_octanol concentration factor 0.885
Carbonate 0.0000 mM
Acidity error -0.44323 mM

18B-28014 Points 30 to 68

M08_octanol concentration factor 1.148
Carbonate 0.0724 mM
Acidity error -0.45335 mM

18B-28014 Points 69 to 110

M08_octanol concentration factor 0.843
Carbonate 0.4970 mM
Acidity error -0.17938 mM

Warnings and errors

Errors None
Warnings None

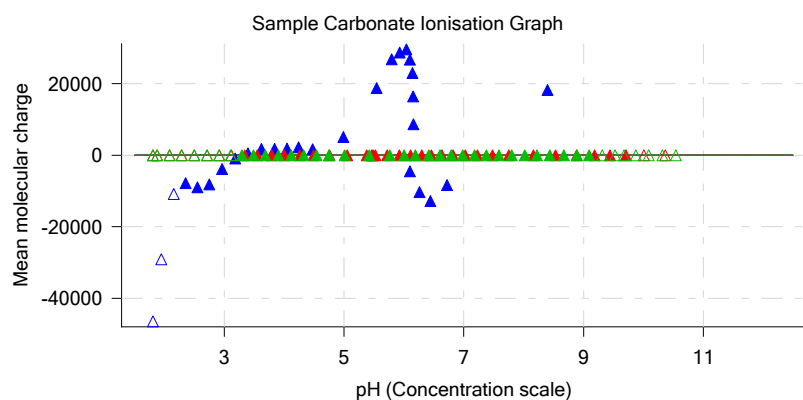
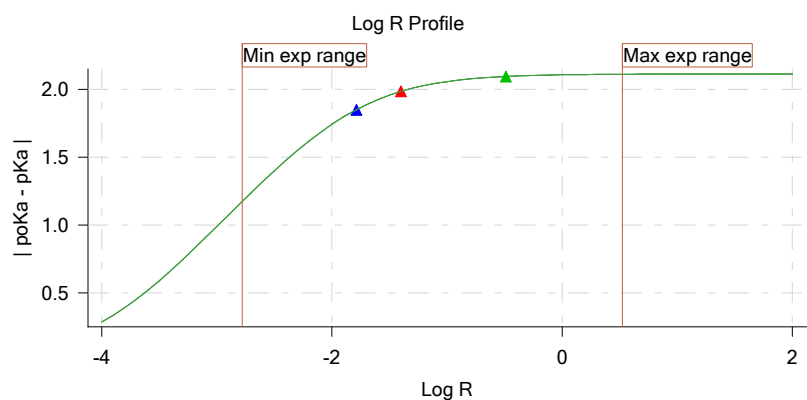
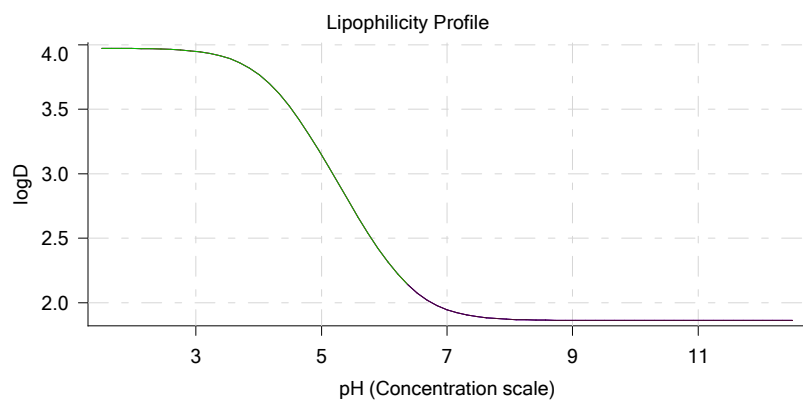
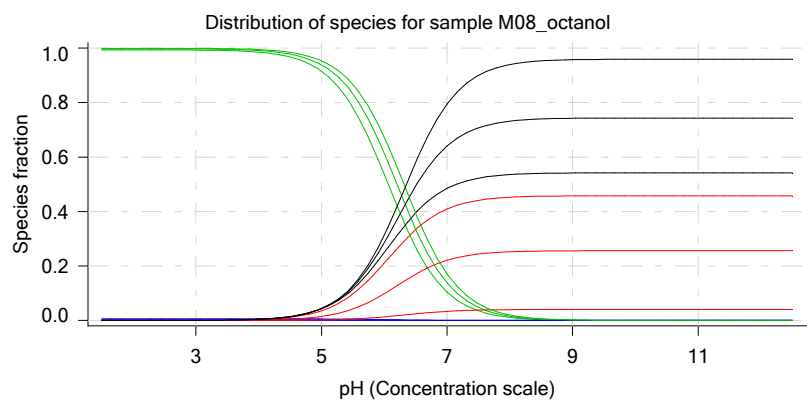
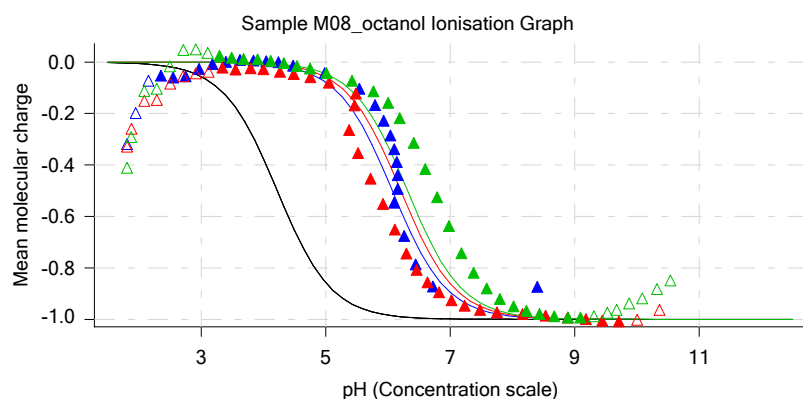
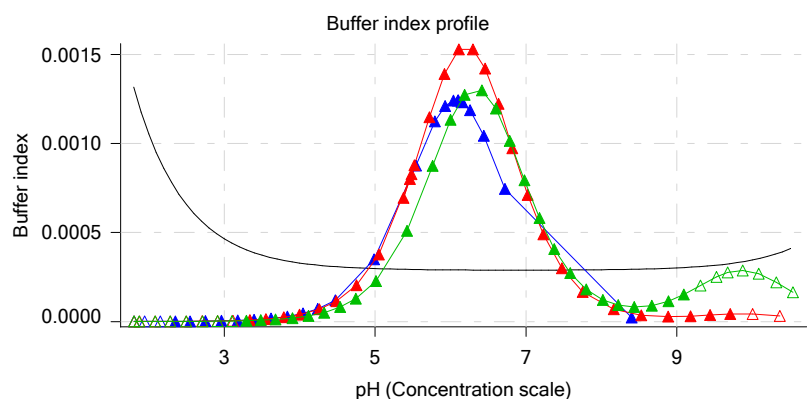
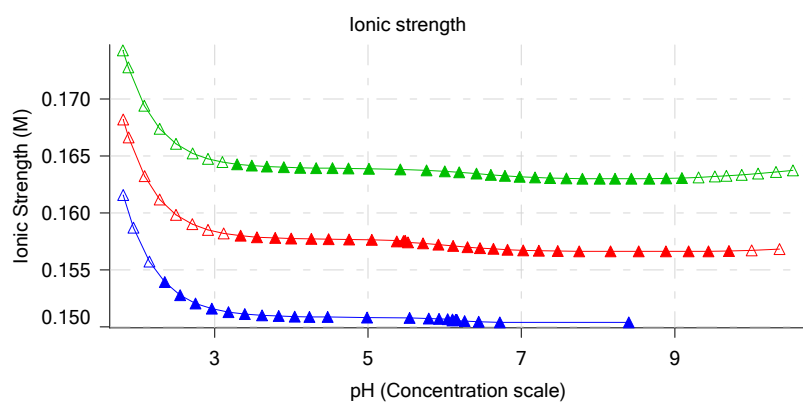
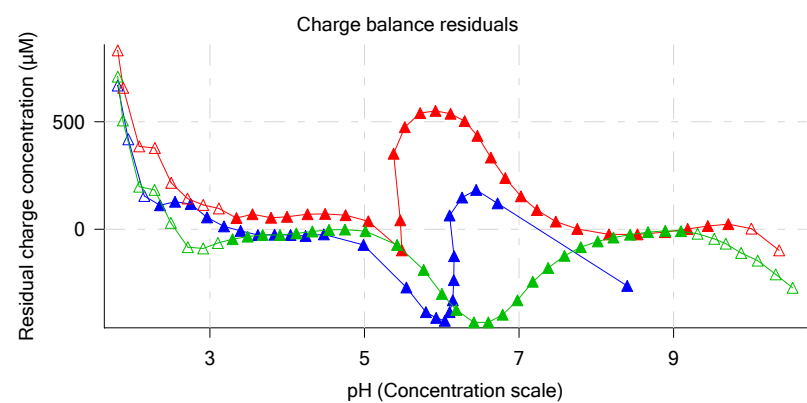
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.97	0.01 %	0.00 %	99.99 %	0.00 %	Stomach pH
1.200	3.97	0.01 %	0.00 %	99.99 %	0.00 %	
2.000	3.97	0.01 %	0.00 %	99.98 %	0.00 %	
3.000	3.95	0.01 %	0.00 %	99.94 %	0.05 %	
4.000	3.77	0.01 %	0.01 %	99.52 %	0.46 %	
5.000	3.15	0.01 %	0.06 %	95.49 %	4.44 %	Blood pH
6.000	2.35	0.01 %	0.43 %	67.96 %	31.59 %	
6.500	2.08	0.00 %	0.81 %	40.15 %	59.03 %	
7.000	1.95	0.00 %	1.12 %	17.50 %	81.37 %	
7.400	1.90	0.00 %	1.25 %	7.79 %	90.96 %	
8.000	1.87	0.00 %	1.33 %	2.08 %	96.59 %	
9.000	1.86	0.00 %	1.35 %	0.21 %	98.43 %	
10.000	1.86	0.00 %	1.36 %	0.02 %	98.62 %	
11.000	1.86	0.00 %	1.36 %	0.00 %	98.64 %	
12.000	1.86	0.00 %	1.36 %	0.00 %	98.64 %	

Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Graphs

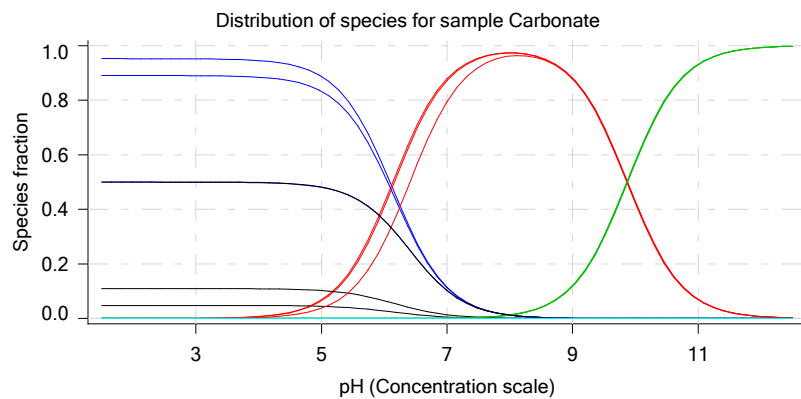




Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28014**
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Experiment start time: **2/28/2018 9:57:03 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18B-28014 Points 2 to 29

Overall results

RMSD 1.233
 Average ionic strength 0.151 M
 Average temperature 24.9°C
 Partition ratio 0.0163 : 1
 Analyte concentration range 2327.5 µM to 2407.5 µM
 Total points considered 25 of 28

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.130 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r

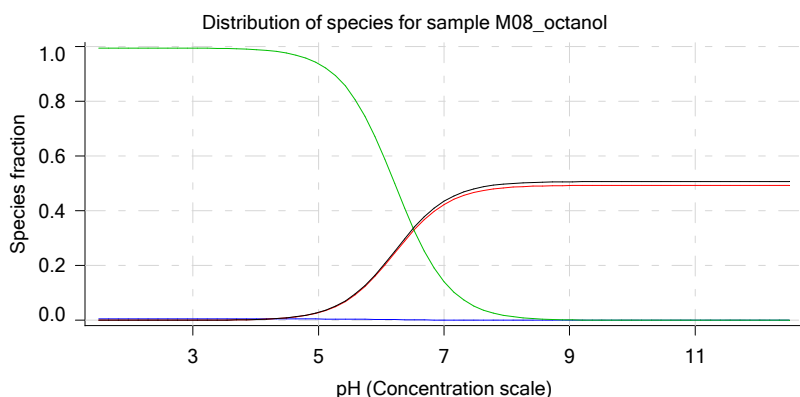
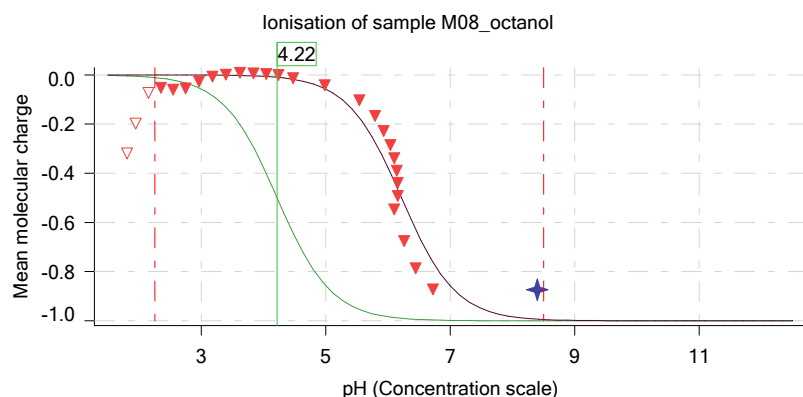
Titrants

0.50 M HCl 0.993513 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 2/28/2018 9:57:03 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor 0.885
 Acid pKa 1 4.22
 logP (neutral XH) 4.09
 logP (X-) 1.80

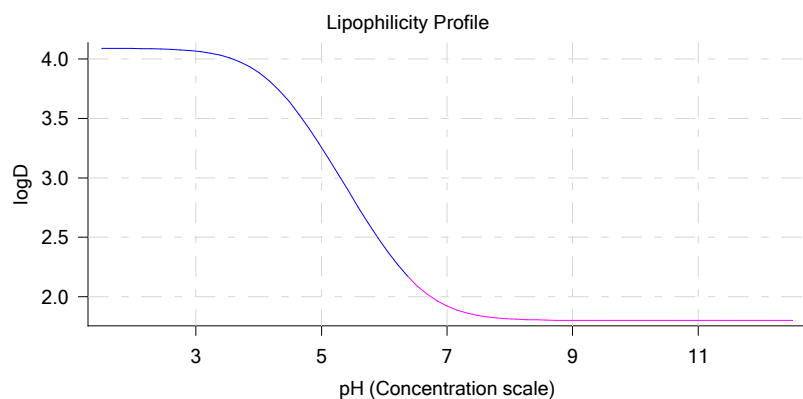
Sample graphs



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



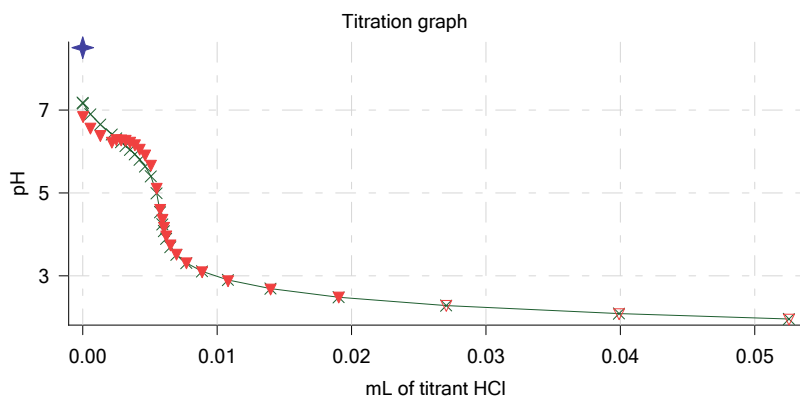
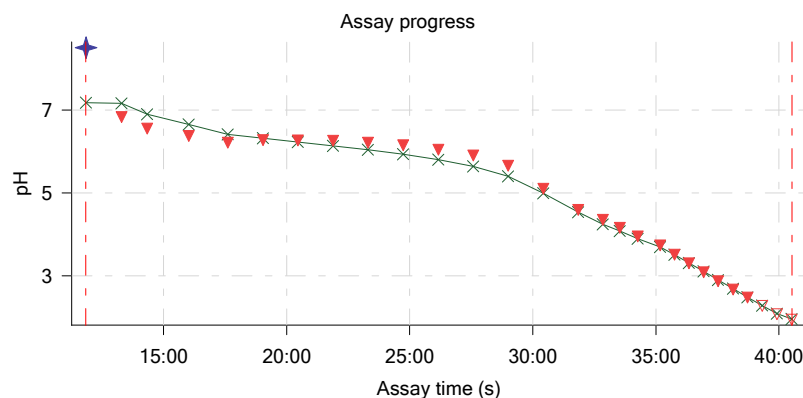
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	4.09	0.49 %	0.00 %	99.50 %	0.00 %	
1.200	4.09	0.49 %	0.00 %	99.50 %	0.00 %	
2.000	4.09	0.49 %	0.00 %	99.50 %	0.00 %	
3.000	4.07	0.49 %	0.03 %	99.44 %	0.03 %	
4.000	3.89	0.49 %	0.30 %	98.91 %	0.30 %	
5.000	3.26	0.47 %	2.81 %	93.83 %	2.89 %	
6.000	2.42	0.31 %	18.58 %	62.00 %	19.11 %	
6.500	2.10	0.17 %	32.38 %	34.16 %	33.29 %	
7.000	1.92	0.07 %	42.31 %	14.12 %	43.50 %	
7.400	1.85	0.03 %	46.26 %	6.14 %	47.56 %	
8.000	1.81	0.01 %	48.51 %	1.62 %	49.87 %	
9.000	1.80	0.00 %	49.23 %	0.16 %	50.61 %	
10.000	1.80	0.00 %	49.30 %	0.02 %	50.68 %	
11.000	1.80	0.00 %	49.31 %	0.00 %	50.69 %	
12.000	1.80	0.00 %	49.31 %	0.00 %	50.69 %	

Carbonate and acidity

Carbonate 0.000 mM
 Acidity error -0.443 mM

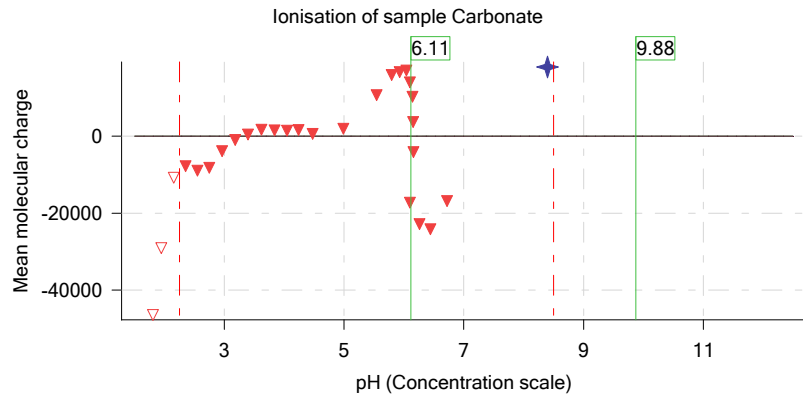
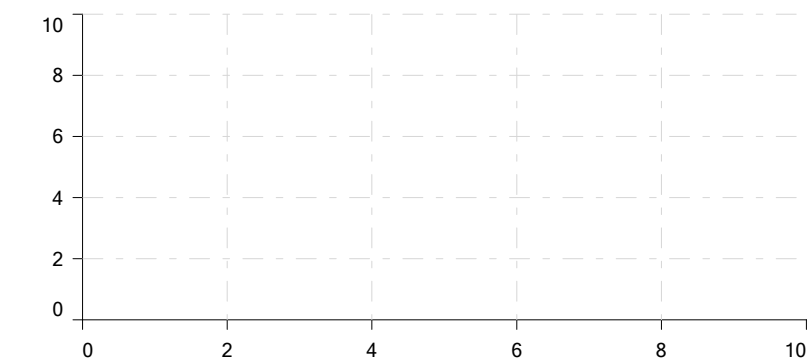
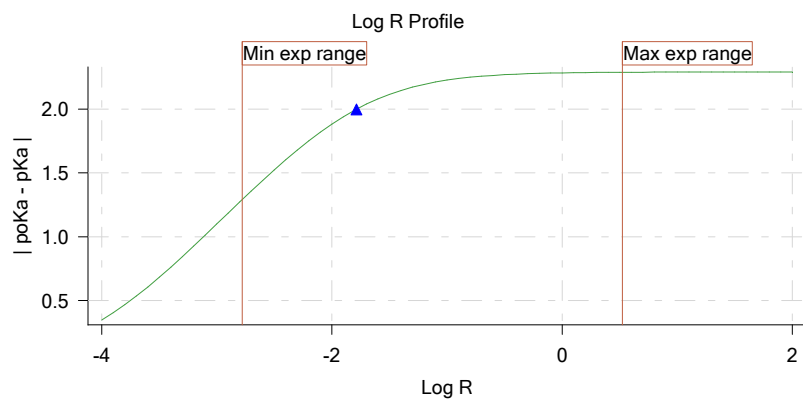
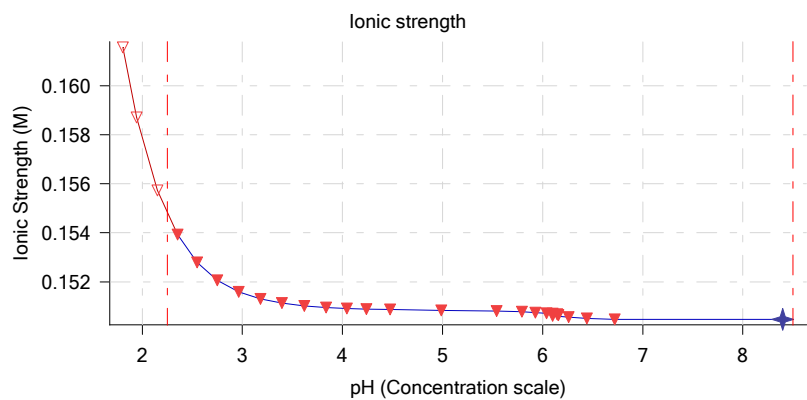
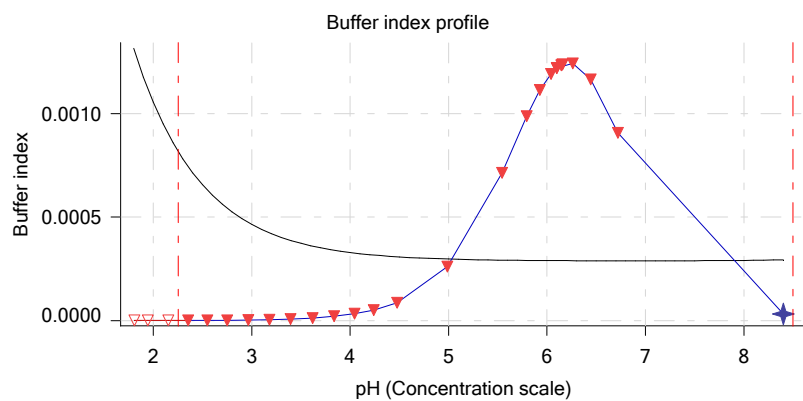
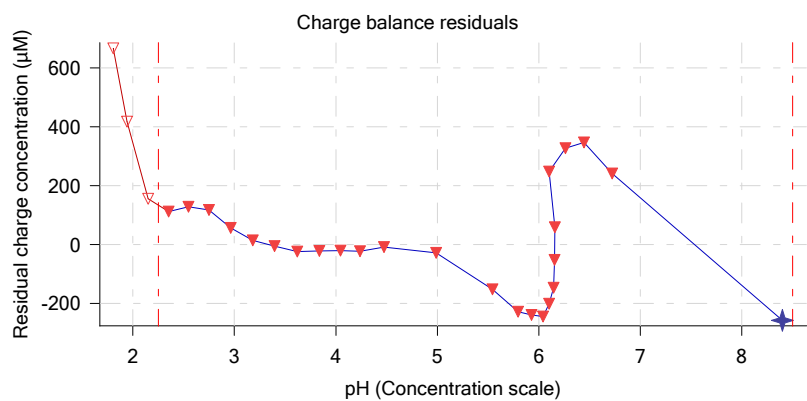
Other graphs



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18B-28014 Points 30 to 68

Overall results

RMSD 0.274
 Average ionic strength 0.157 M
 Average temperature 25.0°C
 Partition ratio 0.0399 : 1
 Analyte concentration range 2118.8 µM to 2194.1 µM
 Total points considered 29 of 39

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.130 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r

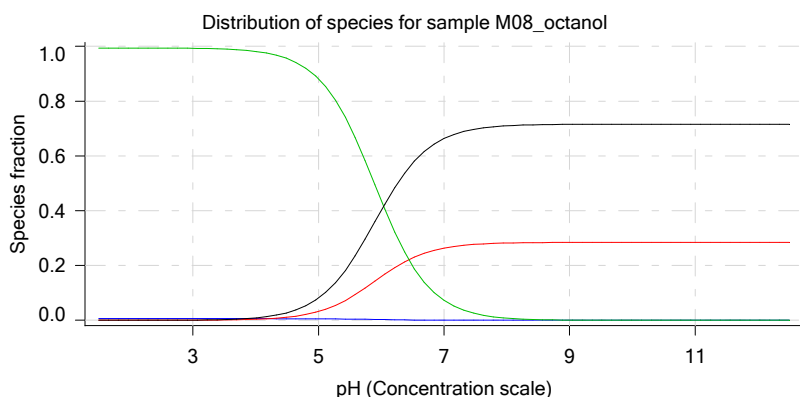
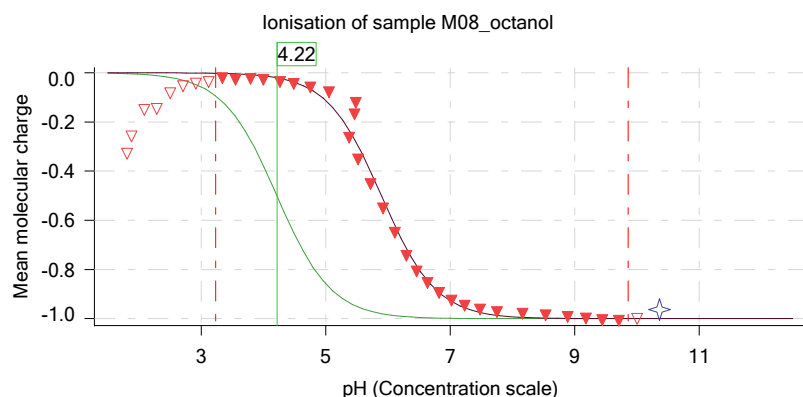
Titrants

0.50 M HCl 0.993513 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 2/28/2018 9:57:03 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor 1.148
 Acid pKa 1 4.22
 logP (neutral XH) 3.62
 logP (X-) 1.80

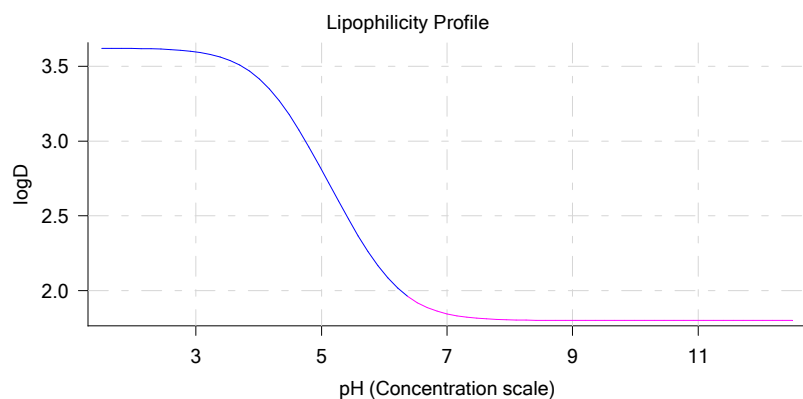
Sample graphs



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



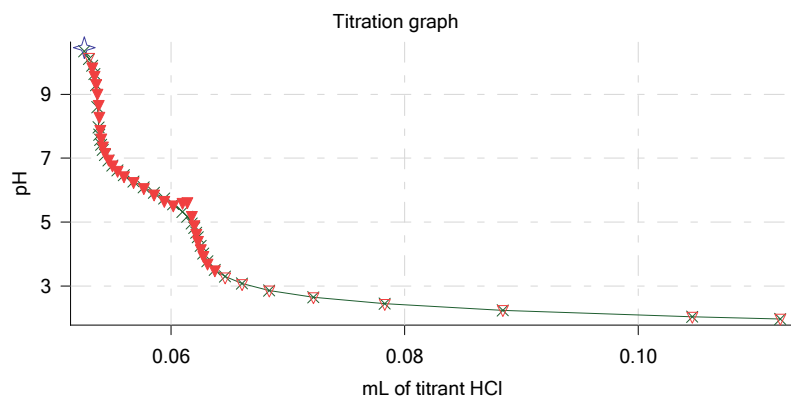
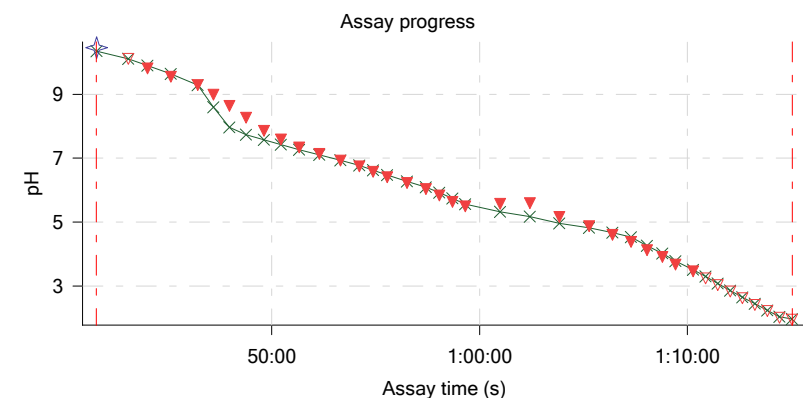
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanolH	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.62	0.59 %	0.00 %	99.40 %	0.00 %	
1.200	3.62	0.59 %	0.00 %	99.40 %	0.00 %	
2.000	3.62	0.59 %	0.00 %	99.39 %	0.01 %	
3.000	3.60	0.59 %	0.04 %	99.28 %	0.09 %	
4.000	3.42	0.59 %	0.35 %	98.17 %	0.89 %	
5.000	2.81	0.53 %	3.18 %	88.28 %	8.01 %	
6.000	2.12	0.26 %	15.85 %	43.97 %	39.91 %	
6.500	1.93	0.12 %	22.73 %	19.93 %	57.22 %	
7.000	1.84	0.04 %	26.34 %	7.31 %	66.31 %	
7.400	1.82	0.02 %	27.56 %	3.04 %	69.38 %	
8.000	1.80	0.00 %	28.21 %	0.78 %	71.01 %	
9.000	1.80	0.00 %	28.41 %	0.08 %	71.51 %	
10.000	1.80	0.00 %	28.43 %	0.01 %	71.56 %	
11.000	1.80	0.00 %	28.43 %	0.00 %	71.57 %	
12.000	1.80	0.00 %	28.43 %	0.00 %	71.57 %	

Carbonate and acidity

Carbonate 0.072 mM
 Acidity error -0.453 mM

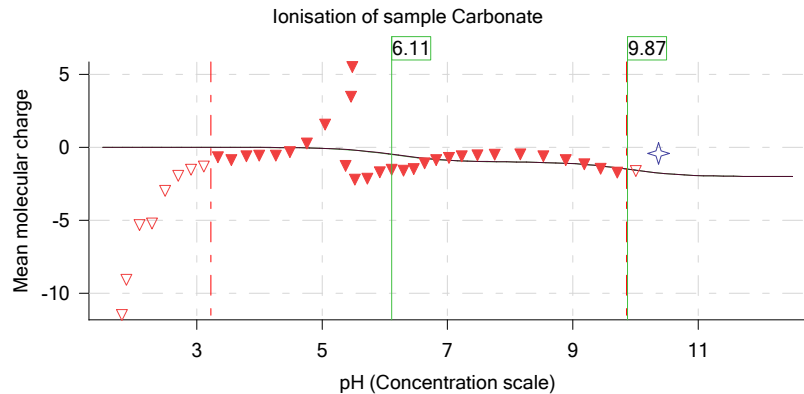
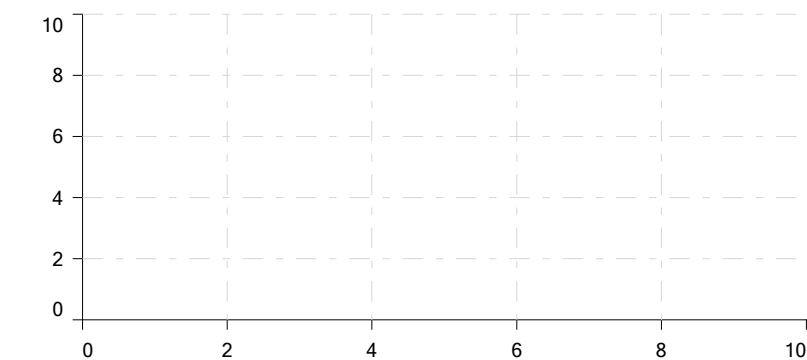
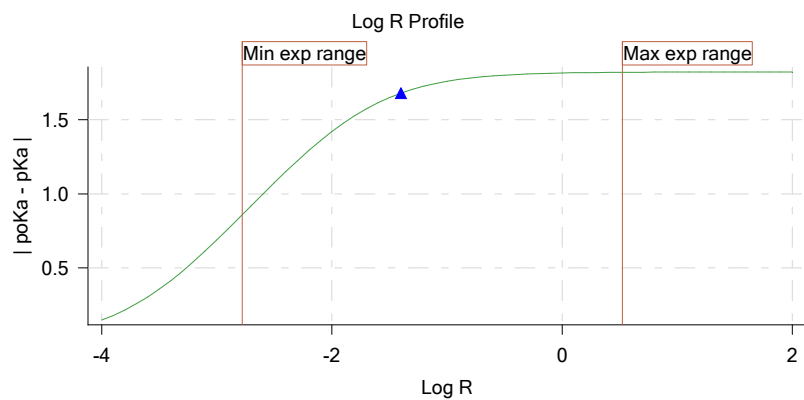
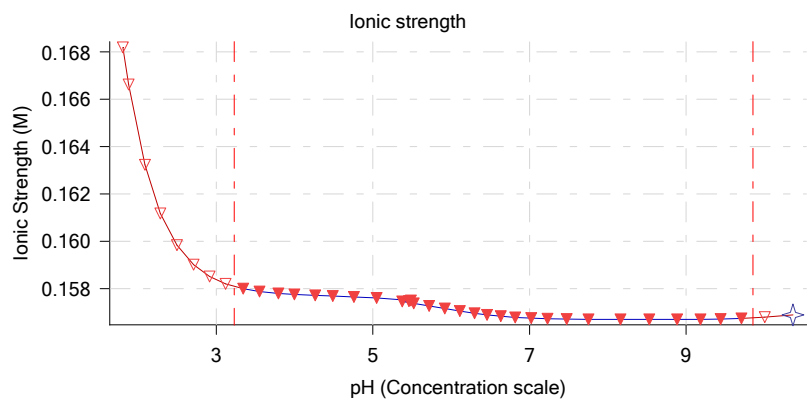
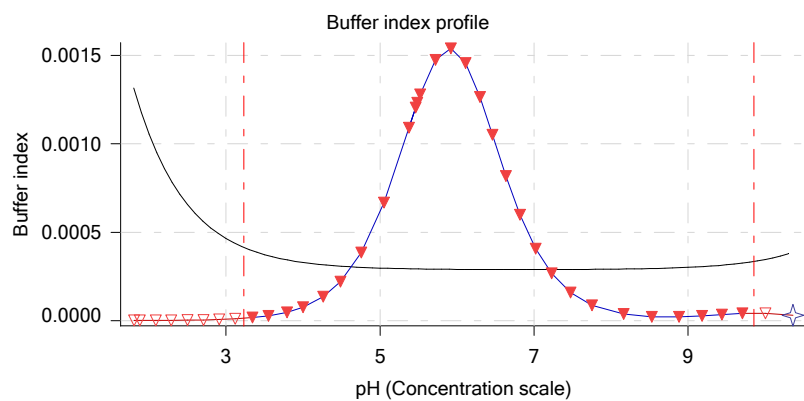
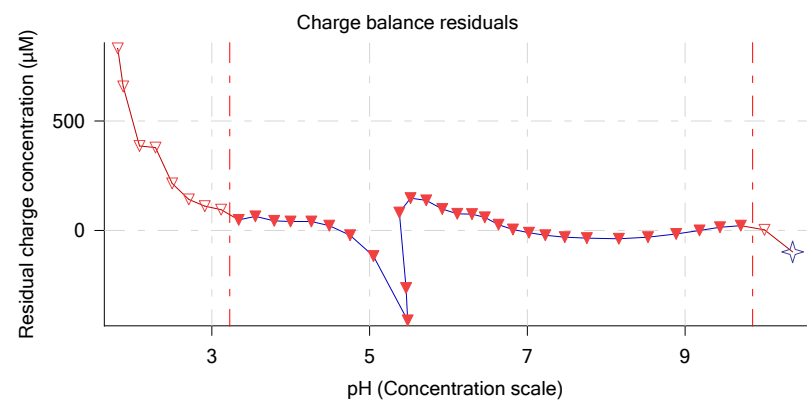
Other graphs



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 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
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Other graphs (continued)



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Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18B-28014 Points 69 to 110

Overall results

RMSD 0.091
 Average ionic strength 0.164 M
 Average temperature 25.0°C
 Partition ratio 0.3243 : 1
 Analyte concentration range 1558.1 µM to 1601.9 µM
 Total points considered 27 of 42

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.130 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r

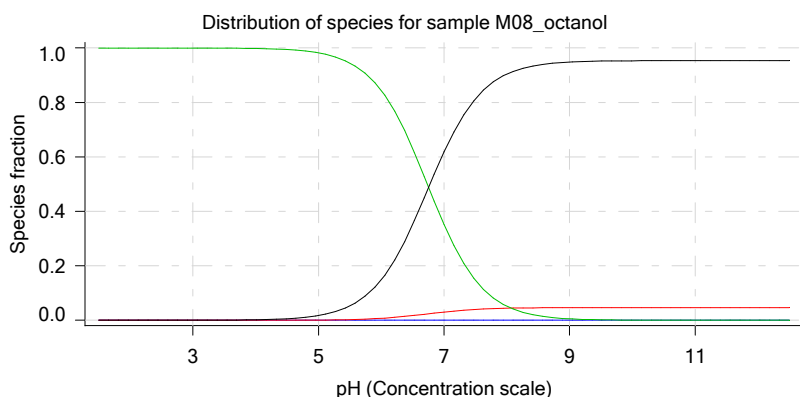
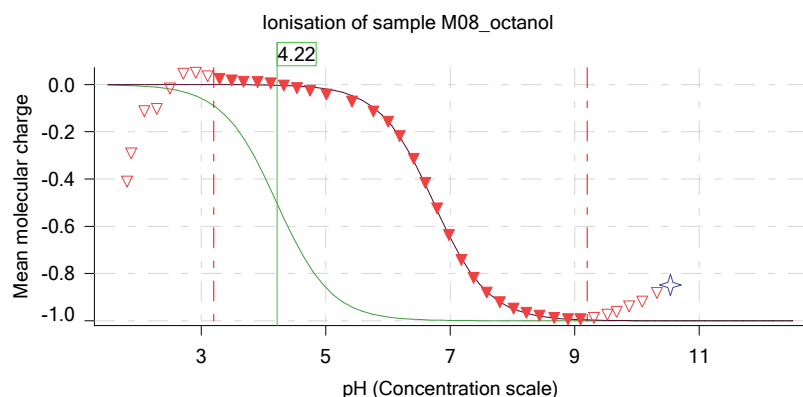
Titrants

0.50 M HCl 0.993513 2/28/2018 9:57:03 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 2/28/2018 9:57:03 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor 0.843
 Acid pKa 1 4.22
 logP (neutral XH) 4.34
 logP (X -) 1.80

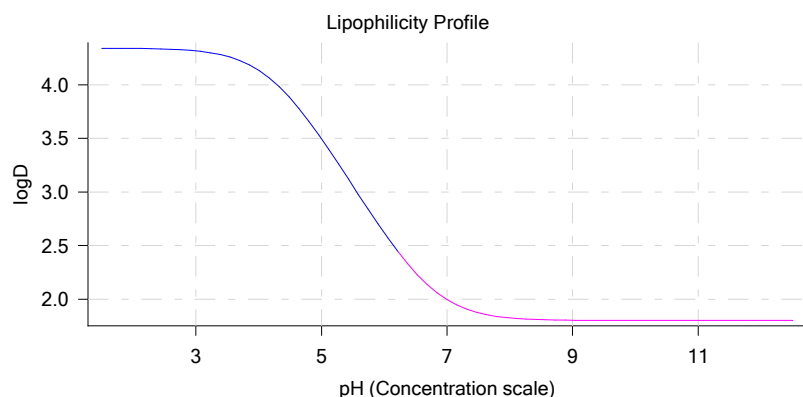
Sample graphs



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 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



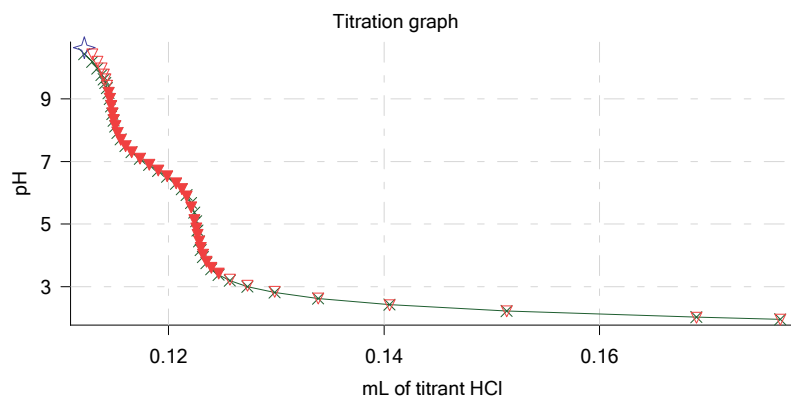
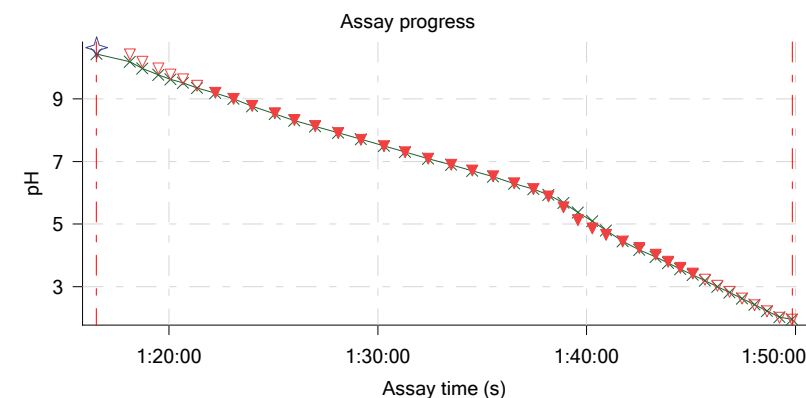
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanolH	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	4.34	0.01 %	0.00 %	99.99 %	0.00 %	
1.200	4.34	0.01 %	0.00 %	99.99 %	0.00 %	
2.000	4.34	0.01 %	0.00 %	99.98 %	0.00 %	
3.000	4.32	0.01 %	0.00 %	99.97 %	0.02 %	
4.000	4.14	0.01 %	0.01 %	99.81 %	0.17 %	
5.000	3.50	0.01 %	0.08 %	98.21 %	1.69 %	
6.000	2.63	0.01 %	0.71 %	84.66 %	14.61 %	
6.500	2.25	0.01 %	1.70 %	63.59 %	34.70 %	
7.000	2.00	0.00 %	3.00 %	35.59 %	61.41 %	
7.400	1.89	0.00 %	3.82 %	18.03 %	78.15 %	
8.000	1.82	0.00 %	4.42 %	5.24 %	90.35 %	
9.000	1.80	0.00 %	4.63 %	0.55 %	94.82 %	
10.000	1.80	0.00 %	4.66 %	0.06 %	95.29 %	
11.000	1.80	0.00 %	4.66 %	0.01 %	95.33 %	
12.000	1.80	0.00 %	4.66 %	0.00 %	95.34 %	

Carbonate and acidity

Carbonate 0.497 mM
 Acidity error -0.179 mM

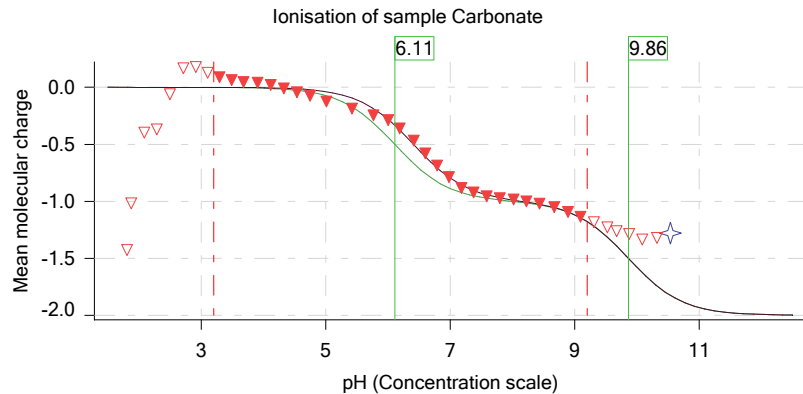
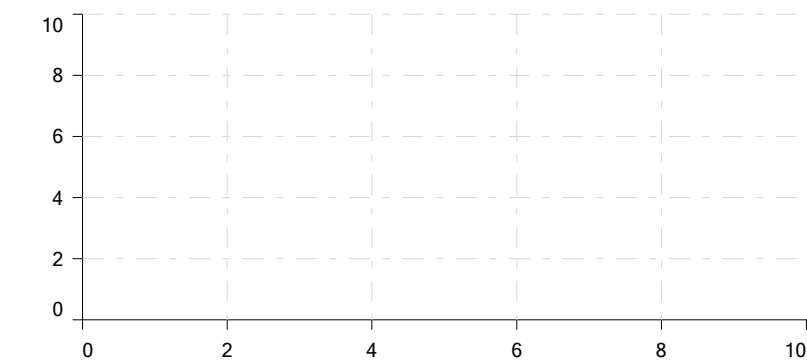
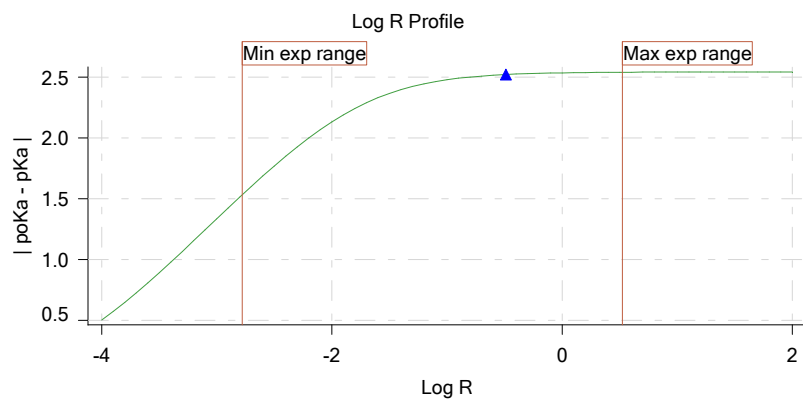
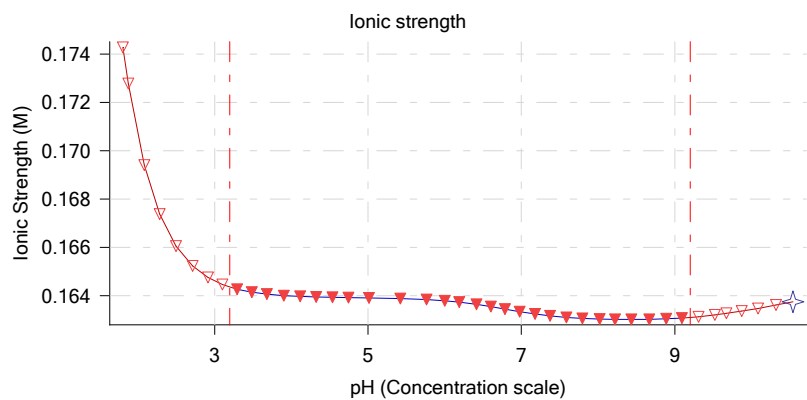
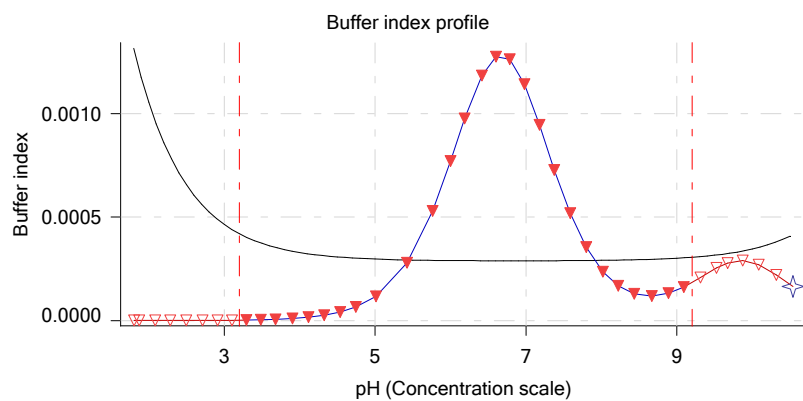
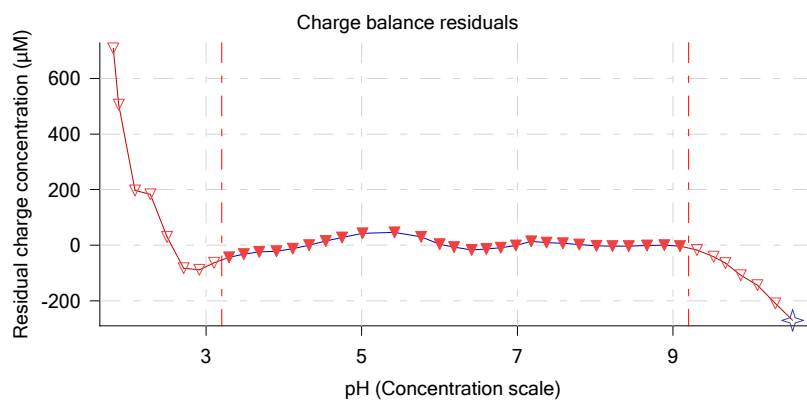
Other graphs



Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)





Assay model

Sample name: **M08_octanol** Experiment start time: **2/28/2018 9:57:03 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18B-28014** Instrument ID: **T312060**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M08_octanol	2/27/2018 5:33:51 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001080 g	2/28/2018 5:24:25 PM	User entered value
Formula weight	293.32 g/mol	2/27/2018 5:33:51 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	293.32	2/27/2018 5:33:51 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 5:33:51 PM	User entered value
Sample is a	Acid	2/27/2018 5:33:51 PM	User entered value
pKa 1	4.22	2/27/2018 5:33:51 PM	User entered value
logP (neutral XH)	3.45	2/28/2018 2:34:15 PM	User entered value
logP (X -)	1.80	2/28/2018 2:34:50 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/time
8:58.1	Manual volume addition				0.02500 mL					
8:59.2	Initial pH = 5.75									
11:51.1	Data point 2	1.50000 mL	0.00000 mL	0.00437 mL	0.02500 mL	8.505	-0.38369	0.99778	0.01897	Time out at 32.0 s
13:17.8	Data point 3	1.50000 mL	0.00002 mL	0.00437 mL	0.02500 mL	6.831	0.01922	0.90141	0.00100	Time out at 32.0 s
14:20.5	Data point 4	1.50000 mL	0.00059 mL	0.00437 mL	0.02500 mL	6.554	0.05114	0.99769	0.00253	Time out at 32.0 s
16:01.3	Data point 5	1.50000 mL	0.00132 mL	0.00437 mL	0.02500 mL	6.372	0.07459	0.99483	0.00369	Time out at 32.0 s
17:37.0	Data point 6	1.50000 mL	0.00216 mL	0.00437 mL	0.02500 mL	6.212	0.09858	0.99770	0.00487	Time out at 32.0 s
19:02.5	Data point 7	1.50000 mL	0.00252 mL	0.00437 mL	0.02500 mL	6.270	0.08713	0.99504	0.00431	Time out at 32.0 s
20:27.8	Data point 8	1.50000 mL	0.00287 mL	0.00437 mL	0.02500 mL	6.267	0.08243	0.99748	0.00408	Time out at 32.0 s
21:53.3	Data point 9	1.50000 mL	0.00320 mL	0.00437 mL	0.02500 mL	6.255	0.08261	0.99774	0.00409	Time out at 32.0 s
23:18.7	Data point 10	1.50000 mL	0.00353 mL	0.00437 mL	0.02500 mL	6.212	0.07670	0.99623	0.00380	Time out at 32.0 s
24:44.1	Data point 11	1.50000 mL	0.00388 mL	0.00437 mL	0.02500 mL	6.152	0.08592	0.99776	0.00425	Time out at 32.0 s
26:09.5	Data point 12	1.50000 mL	0.00426 mL	0.00437 mL	0.02500 mL	6.040	0.08353	0.99742	0.00413	Time out at 32.0 s
27:34.9	Data point 13	1.50000 mL	0.00466 mL	0.00437 mL	0.02500 mL	5.906	0.08469	0.99736	0.00419	Time out at 32.0 s
29:00.3	Data point 14	1.50000 mL	0.00508 mL	0.00437 mL	0.02500 mL	5.655	0.08514	0.99629	0.00421	Time out at 32.0 s



Assay Events

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28014**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
30:25.6	Data point 15	1.50000 mL	0.00550 mL	0.00437 mL	0.02500 mL	5.102	0.04617	0.99374	0.00229	Timed out at 59.5 s
31:51.0	Data point 16	1.50000 mL	0.00576 mL	0.00437 mL	0.02500 mL	4.592	0.01831	0.87650	0.00097	24.0 s
32:50.6	Data point 17	1.50000 mL	0.00593 mL	0.00437 mL	0.02500 mL	4.356	0.01879	0.87405	0.00099	16.0 s
33:32.0	Data point 18	1.50000 mL	0.00604 mL	0.00437 mL	0.02500 mL	4.163	0.01848	0.95772	0.00093	13.5 s
34:16.1	Data point 19	1.50000 mL	0.00623 mL	0.00437 mL	0.02500 mL	3.955	0.01959	0.95038	0.00099	13.0 s
35:10.1	Data point 20	1.50000 mL	0.00654 mL	0.00437 mL	0.02500 mL	3.739	0.01840	0.93630	0.00094	10.0 s
35:45.5	Data point 21	1.50000 mL	0.00698 mL	0.00437 mL	0.02500 mL	3.515	0.01107	0.91474	0.00057	10.0 s
36:20.9	Data point 22	1.50000 mL	0.00771 mL	0.00437 mL	0.02500 mL	3.301	-0.00792	0.20574	0.00086	10.0 s
36:56.3	Data point 23	1.50000 mL	0.00889 mL	0.00437 mL	0.02500 mL	3.086	-0.00002	0.00010	0.00009	10.0 s
37:31.8	Data point 24	1.50000 mL	0.01082 mL	0.00437 mL	0.02500 mL	2.873	-0.00479	0.63485	0.00030	10.5 s
38:07.8	Data point 25	1.50000 mL	0.01399 mL	0.00437 mL	0.02500 mL	2.674	-0.01143	0.54403	0.00077	10.0 s
38:43.4	Data point 26	1.50000 mL	0.01905 mL	0.00437 mL	0.02500 mL	2.478	-0.01045	0.80609	0.00057	10.0 s
39:19.0	Data point 27	1.50000 mL	0.02705 mL	0.00437 mL	0.02500 mL	2.280	-0.01095	0.68427	0.00065	10.0 s
39:54.7	Data point 28	1.50000 mL	0.03991 mL	0.00437 mL	0.02500 mL	2.076	-0.01774	0.88391	0.00093	10.5 s
40:31.0	Data point 29	1.50000 mL	0.05256 mL	0.00437 mL	0.02500 mL	1.944	-0.01689	0.91021	0.00087	10.0 s
41:34.8	Data point 30	1.50000 mL	0.05256 mL	0.06058 mL	0.06500 mL	10.463	0.01671	0.80475	0.00092	55.5 s
43:06.2	Data point 31	1.50000 mL	0.05299 mL	0.06058 mL	0.06500 mL	10.105	-0.00088	0.00194	0.00098	30.0 s
44:01.6	Data point 32	1.50000 mL	0.05325 mL	0.06058 mL	0.06500 mL	9.808	-0.01675	0.76998	0.00094	37.0 s
45:09.2	Data point 33	1.50000 mL	0.05343 mL	0.06058 mL	0.06500 mL	9.543	-0.01717	0.74125	0.00098	41.5 s
46:26.4	Data point 34	1.50000 mL	0.05357 mL	0.06058 mL	0.06500 mL	9.285	-0.00869	0.87535	0.00046	10.0 s
47:12.0	Data point 35	1.50000 mL	0.05369 mL	0.06058 mL	0.06500 mL	8.988	0.00397	0.06470	0.00077	10.0 s
47:57.7	Data point 36	1.50000 mL	0.05379 mL	0.06058 mL	0.06500 mL	8.634	0.01554	0.63385	0.00096	13.0 s
48:46.3	Data point 37	1.50000 mL	0.05386 mL	0.06058 mL	0.06500 mL	8.268	0.01699	0.72054	0.00099	16.0 s
49:38.0	Data point 38	1.50000 mL	0.05393 mL	0.06058 mL	0.06500 mL	7.860	0.01563	0.77436	0.00088	18.0 s
50:26.5	Data point 39	1.50000 mL	0.05402 mL	0.06058 mL	0.06500 mL	7.583	0.01366	0.60795	0.00087	17.5 s
51:19.7	Data point 40	1.50000 mL	0.05416 mL	0.06058 mL	0.06500 mL	7.337	0.01707	0.87652	0.00090	17.5 s
52:18.0	Data point 41	1.50000 mL	0.05435 mL	0.06058 mL	0.06500 mL	7.132	0.01352	0.65718	0.00082	15.0 s
53:19.0	Data point 42	1.50000 mL	0.05463 mL	0.06058 mL	0.06500 mL	6.929	0.01590	0.72033	0.00093	18.0 s
54:12.7	Data point 43	1.50000 mL	0.05499 mL	0.06058 mL	0.06500 mL	6.745	0.01686	0.80981	0.00093	15.0 s
54:53.1	Data point 44	1.50000 mL	0.05541 mL	0.06058 mL	0.06500 mL	6.570	0.01319	0.58565	0.00085	15.0 s
55:33.5	Data point 45	1.50000 mL	0.05597 mL	0.06058 mL	0.06500 mL	6.408	0.01755	0.91751	0.00090	16.0 s
56:30.4	Data point 46	1.50000 mL	0.05680 mL	0.06058 mL	0.06500 mL	6.222	0.01824	0.88012	0.00096	14.0 s
57:25.4	Data point 47	1.50000 mL	0.05767 mL	0.06058 mL	0.06500 mL	6.032	0.01601	0.70284	0.00094	13.0 s
58:03.8	Data point 48	1.50000 mL	0.05854 mL	0.06058 mL	0.06500 mL	5.832	0.01586	0.73469	0.00091	12.0 s
58:41.4	Data point 49	1.50000 mL	0.05941 mL	0.06058 mL	0.06500 mL	5.634	0.01736	0.78548	0.00097	12.0 s
59:18.8	Data point 50	1.50000 mL	0.06018 mL	0.06058 mL	0.06500 mL	5.490	0.10872	0.99860	0.00537	Timed out at 59.5 s
1:00:59.7	Data point 51	1.50000 mL	0.06098 mL	0.06058 mL	0.06500 mL	5.576	0.16163	0.99800	0.00799	Timed out at 59.5 s
1:02:25.1	Data point 52	1.50000 mL	0.06138 mL	0.06058 mL	0.06500 mL	5.597	0.09780	0.99796	0.00484	Timed out at 59.5 s
1:03:50.6	Data point 53	1.50000 mL	0.06178 mL	0.06058 mL	0.06500 mL	5.164	0.03874	0.98187	0.00193	Timed out at 59.5 s
1:05:15.9	Data point 54	1.50000 mL	0.06199 mL	0.06058 mL	0.06500 mL	4.871	0.01890	0.95104	0.00096	37.5 s
1:06:24.0	Data point 55	1.50000 mL	0.06216 mL	0.06058 mL	0.06500 mL	4.605	0.02009	0.98775	0.00100	22.5 s
1:07:17.2	Data point 56	1.50000 mL	0.06230 mL	0.06058 mL	0.06500 mL	4.379	0.01733	0.86039	0.00092	15.5 s
1:08:03.2	Data point 57	1.50000 mL	0.06254 mL	0.06058 mL	0.06500 mL	4.117	0.01748	0.84391	0.00094	14.0 s
1:08:47.7	Data point 58	1.50000 mL	0.06277 mL	0.06058 mL	0.06500 mL	3.910	0.01951	0.98119	0.00097	12.5 s
1:09:25.6	Data point 59	1.50000 mL	0.06312 mL	0.06058 mL	0.06500 mL	3.670	0.01603	0.74774	0.00092	10.0 s
1:10:16.5	Data point 60	1.50000 mL	0.06376 mL	0.06058 mL	0.06500 mL	3.462	0.00750	0.80522	0.00041	10.0 s
1:10:52.0	Data point 61	1.50000 mL	0.06463 mL	0.06058 mL	0.06500 mL	3.238	-0.00145	0.00710	0.00085	10.0 s
1:11:27.4	Data point 62	1.50000 mL	0.06609 mL	0.06058 mL	0.06500 mL	3.035	-0.00146	0.02277	0.00048	10.5 s
1:12:03.4	Data point 63	1.50000 mL	0.06841 mL	0.06058 mL	0.06500 mL	2.831	-0.00808	0.27293	0.00076	10.0 s
1:12:38.9	Data point 64	1.50000 mL	0.07218 mL	0.06058 mL	0.06500 mL	2.624	-0.00574	0.80349	0.00032	10.0 s
1:13:14.6	Data point 65	1.50000 mL	0.07832 mL	0.06058 mL	0.06500 mL	2.413	-0.00805	0.73778	0.00046	10.0 s
1:13:50.2	Data point 66	1.50000 mL	0.08841 mL	0.06058 mL	0.06500 mL	2.216	-0.00955	0.79291	0.00053	10.0 s

Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:14:26.0	Data point 67	1.50000 mL	0.10463 mL	0.06058 mL	0.06500 mL	2.013	-0.01476	0.90024	0.00077	10.0 s
1:15:01.6	Data point 68	1.50000 mL	0.11218 mL	0.06058 mL	0.06500 mL	1.944	-0.00748	0.85449	0.00040	10.0 s
1:16:32.0	Data point 69	1.50000 mL	0.11218 mL	0.12131 mL	0.56500 mL	10.638	-0.02692	0.97300	0.00135	Timed out at 59.5 s
1:18:07.8	Data point 70	1.50000 mL	0.11291 mL	0.12131 mL	0.56500 mL	10.418	-0.01629	0.90234	0.00085	10.5 s
1:18:43.7	Data point 71	1.50000 mL	0.11341 mL	0.12131 mL	0.56500 mL	10.185	-0.00481	0.66052	0.00029	10.0 s
1:19:29.4	Data point 72	1.50000 mL	0.11378 mL	0.12131 mL	0.56500 mL	9.973	0.00415	0.69795	0.00025	10.0 s
1:20:04.7	Data point 73	1.50000 mL	0.11399 mL	0.12131 mL	0.56500 mL	9.775	0.00051	0.00415	0.00039	10.0 s
1:20:40.0	Data point 74	1.50000 mL	0.11414 mL	0.12131 mL	0.56500 mL	9.625	0.01049	0.80316	0.00058	10.0 s
1:21:20.4	Data point 75	1.50000 mL	0.11430 mL	0.12131 mL	0.56500 mL	9.413	0.01849	0.91674	0.00095	16.5 s
1:22:12.7	Data point 76	1.50000 mL	0.11444 mL	0.12131 mL	0.56500 mL	9.196	0.01358	0.49556	0.00095	17.5 s
1:23:05.8	Data point 77	1.50000 mL	0.11456 mL	0.12131 mL	0.56500 mL	8.994	0.01898	0.97137	0.00095	12.0 s
1:23:58.6	Data point 78	1.50000 mL	0.11468 mL	0.12131 mL	0.56500 mL	8.773	0.00423	0.05467	0.00089	19.5 s
1:25:04.0	Data point 79	1.50000 mL	0.11479 mL	0.12131 mL	0.56500 mL	8.540	0.01751	0.95118	0.00089	15.5 s
1:26:00.5	Data point 80	1.50000 mL	0.11491 mL	0.12131 mL	0.56500 mL	8.327	0.00999	0.26899	0.00095	18.5 s
1:26:59.9	Data point 81	1.50000 mL	0.11505 mL	0.12131 mL	0.56500 mL	8.125	0.00630	0.12857	0.00087	20.0 s
1:28:05.9	Data point 82	1.50000 mL	0.11526 mL	0.12131 mL	0.56500 mL	7.904	0.00961	0.25771	0.00093	19.5 s
1:29:11.3	Data point 83	1.50000 mL	0.11557 mL	0.12131 mL	0.56500 mL	7.692	0.01317	0.53307	0.00089	20.5 s
1:30:17.8	Data point 84	1.50000 mL	0.11602 mL	0.12131 mL	0.56500 mL	7.484	0.01066	0.33152	0.00091	19.5 s
1:31:18.1	Data point 85	1.50000 mL	0.11658 mL	0.12131 mL	0.56500 mL	7.286	0.01482	0.73005	0.00086	20.5 s
1:32:24.8	Data point 86	1.50000 mL	0.11736 mL	0.12131 mL	0.56500 mL	7.089	0.01351	0.56423	0.00089	19.5 s
1:33:30.4	Data point 87	1.50000 mL	0.11820 mL	0.12131 mL	0.56500 mL	6.896	0.01748	0.83538	0.00095	20.0 s
1:34:31.3	Data point 88	1.50000 mL	0.11905 mL	0.12131 mL	0.56500 mL	6.712	0.01401	0.48910	0.00099	19.0 s
1:35:31.3	Data point 89	1.50000 mL	0.11987 mL	0.12131 mL	0.56500 mL	6.525	0.00912	0.22976	0.00094	19.5 s
1:36:31.7	Data point 90	1.50000 mL	0.12070 mL	0.12131 mL	0.56500 mL	6.300	0.01131	0.37052	0.00092	19.5 s
1:37:27.0	Data point 91	1.50000 mL	0.12124 mL	0.12131 mL	0.56500 mL	6.113	0.01242	0.37784	0.00100	17.5 s
1:38:09.9	Data point 92	1.50000 mL	0.12168 mL	0.12131 mL	0.56500 mL	5.877	0.01326	0.59032	0.00085	18.0 s
1:38:53.3	Data point 93	1.50000 mL	0.12211 mL	0.12131 mL	0.56500 mL	5.536	0.01531	0.70704	0.00090	16.5 s
1:39:35.3	Data point 94	1.50000 mL	0.12241 mL	0.12131 mL	0.56500 mL	5.126	0.01004	0.33249	0.00086	15.5 s
1:40:16.1	Data point 95	1.50000 mL	0.12258 mL	0.12131 mL	0.56500 mL	4.862	0.01660	0.85540	0.00089	14.0 s
1:40:55.6	Data point 96	1.50000 mL	0.12270 mL	0.12131 mL	0.56500 mL	4.655	0.01286	0.68795	0.00077	12.5 s
1:41:43.7	Data point 97	1.50000 mL	0.12284 mL	0.12131 mL	0.56500 mL	4.442	0.01567	0.70157	0.00092	12.0 s
1:42:31.3	Data point 98	1.50000 mL	0.12300 mL	0.12131 mL	0.56500 mL	4.233	0.00457	0.07507	0.00082	11.0 s
1:43:17.9	Data point 99	1.50000 mL	0.12321 mL	0.12131 mL	0.56500 mL	4.023	0.01009	0.34406	0.00085	10.5 s
1:43:53.8	Data point 100	1.50000 mL	0.12352 mL	0.12131 mL	0.56500 mL	3.800	0.00859	0.33185	0.00074	10.0 s
1:44:29.3	Data point 101	1.50000 mL	0.12397 mL	0.12131 mL	0.56500 mL	3.606	0.01096	0.49543	0.00077	10.0 s
1:45:04.7	Data point 102	1.50000 mL	0.12465 mL	0.12131 mL	0.56500 mL	3.415	-0.00112	0.00437	0.00083	10.0 s
1:45:40.2	Data point 103	1.50000 mL	0.12571 mL	0.12131 mL	0.56500 mL	3.225	-0.00516	0.50756	0.00036	10.0 s
1:46:15.7	Data point 104	1.50000 mL	0.12733 mL	0.12131 mL	0.56500 mL	3.035	0.00000	0.00000	0.00038	10.0 s
1:46:51.1	Data point 105	1.50000 mL	0.12984 mL	0.12131 mL	0.56500 mL	2.835	-0.01164	0.95088	0.00059	10.0 s
1:47:26.7	Data point 106	1.50000 mL	0.13389 mL	0.12131 mL	0.56500 mL	2.621	-0.00308	0.11765	0.00044	10.0 s
1:48:02.3	Data point 107	1.50000 mL	0.14052 mL	0.12131 mL	0.56500 mL	2.411	-0.01254	0.94329	0.00064	10.0 s
1:48:38.0	Data point 108	1.50000 mL	0.15139 mL	0.12131 mL	0.56500 mL	2.215	-0.01773	0.98451	0.00088	10.0 s
1:49:13.9	Data point 109	1.50000 mL	0.16900 mL	0.12131 mL	0.56500 mL	2.009	-0.01817	0.96311	0.00091	10.5 s
1:49:50.1	Data point 110	1.50000 mL	0.17679 mL	0.12131 mL	0.56500 mL	1.942	-0.01341	0.97758	0.00067	10.5 s
1:50:09.6	Assay volumes	1.50000 mL	0.17679 mL	0.12131 mL	0.56500 mL					



Sample name: **M08_octanol** Experiment start time: **2/28/2018 9:57:03 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18B-28014** Instrument ID: **T312060**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.025 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	High to low pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.040 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			



Assay Settings

Sample name: **M08_octanol** Experiment start time: **2/28/2018 9:57:03 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18B-28014** Instrument ID: **T312060**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.500 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	2/28/2018 9:57:03 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	2/28/2018 9:57:03 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	2/28/2018 9:57:03 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	2/28/2018 9:57:03 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	2/28/2018 9:57:03 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	2/28/2018 9:57:03 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 11:05:59 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 11:27:22 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 11:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 10:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M08_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18B-28014**
 Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 9:57:03 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titration		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+3.66 mV		2/28/2018 9:57:31 PM
Filling solution	3M KCl	KCL097	2/27/2018 10:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 11:23:32 AM
Wash 2	0.5% Triton X-100 in H2O		2/28/2018 11:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 11:24:06 AM
Buffer position 2	pH 7		2/28/2018 11:24:08 AM
Storage position			2/28/2018 11:21:14 AM
Wash water	8.7e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	6.8e+003 mL		11/28/2017 11:36:29 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M08_octanol** Experiment start time: **2/28/2018 9:57:03 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18B-28014** Instrument ID: **T312060**
Filename: **G:\OpenLab_PFA_Sirius-T3-2\Data2018\18B-28014_M08_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00